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Hamiltonian Structure of a Solution Strategy for the Semi-Geostrophic Equations

by

I. Roulstone and J. Norbury

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I. Roulstone

Short-Range Forecasting Research Division
Meteorological Office
London Road
Bracknell
Berkshire. RG12 2SZ.

J. Norbury

Mathematical Institute
24-29 St. Giles
Oxford. OX1 3LB.

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Abstract

A canonical structure for the semi-geostrophic equations is presented and from this, a reduced, noncanonical and formally Hamiltonian approach to an algorithm for integrating the equations of motion is formulated. Basic functional methods are introduced and the Lagrangian and Eulerian kinematic structures are discussed.

1 Introduction.

The use of Hamiltonian methods in fluid dynamics has become the fashion in recent years as they enable one to use methods of analytical mechanics (as opposed to methods of vector analysis), in formulating the equations of motion and giving insights, in particular, to the relationships between the underlying kinematics and the dynamics of the fluid. They may be especially important in atmospheric dynamics for a variety of reasons. The existence of a relationship between symmetries and conservation laws (Noether's theorem); the Lagrangian and Eulerian formulation of the kinematics and the numerical integration of the equations of motion are all contemporary subjects of significant interest to the theorist and modeller. Studies using *filtered* or *balanced* models are essential to describing flow regimes that dominate certain spatial or temporal scales. In these cases the Hamiltonian approach offers a systematic method for studying, for example, the conservation laws and related symmetries of the model. Recently (Salmon (1988a)) it has been proposed that *Generalized* Hamiltonian methods, developed by Dirac (1958), may help in understanding the nature of the approximations used to obtain these balanced models, thus complementing scale analysis.

Despite fundamental advances in Hamiltonian formulations of fluid dynamics there remain many open problems that concern, in particular, the theorist in geophysical studies. Some of these questions relate to the structure of the balanced models mentioned above, but in addition, Eulerian formulations of the equations of motion, of central importance to numerical models, also require further extensive re-

search. In particular the application of ideas from abstract approaches to the subject (see for example, Arnol'd (1989), appendix 2; Marsden & Weinstein (1983)) need to be applied to specific models. As an example of the (often surprising) features that emerge, consider the hydrostatic approximation to 3-dimensional, incompressible, rotating, adiabatic flow (Holm & Long (1989)). This does not appear as a straightforward approximation to the Hamiltonian version of the nonhydrostatic model (Shepherd (1990)). For recent reviews of the subject see Salmon (1988b) and Shepherd (1990). The reader should therefore not be surprised to find papers devoted to the Hamiltonian formulation of 2- and 3-dimensional models that have been established subjects in standard textbooks for some time.

In this paper we will be concerned with a 3-dimensional version of the semi-geostrophic (SG) equations (Hoskins & Draghici (1977)). The motivation for this work comes primarily from the formulation of the equations of motion in numerical models. Hoskins and Bretherton (1972) showed that the SG equations may be expressed in terms of Lagrangian conservation laws and Cullen *et. al.* (1987) have developed a numerical model (the so-called *geometric model*) which represents the fluid as a finite collection of parcels with conserved momentum and thermodynamic labels. A stable manifold within the dynamical system of the atmosphere may be defined by using a convexity principle to minimise the energy. An extra advantage of this principle is that it applies to variables which have discontinuities. It is not our purpose here to discuss the *dynamics* of either SG theory or the geometric model, but rather the *kinematics*. Salmon (1985) and Shutts (1989) have obtained versions of the SG equations from Hamilton's Principle - a statement equivalent to

Newton's laws of motion. This approach is based on essentially Lagrangian kinematics (in the sense of position/velocity space), whereas the basis of this study is manifestly Hamiltonian. Here we are concerned with Lagrangian (in the sense of particle labelling coordinates) and Eulerian formulations of the equations, however we will not concern ourselves with a derivation of the equations. Recent developments in the numerical integration of Hamiltonian systems has emphasized the importance of preserving kinematic structure in solution strategies for these models. We will pay particular attention to this structure as the SG equations of motion may be written either as a set of coupled ordinary differential equations or, as in the formulation of the geometric model, an advection equation based on a *nonlinear vorticity/streamfunction system.* In this latter case the Monge-Ampere equation replaces the usual "vorticity equals Laplacian of streamfunction" relationship. The Hamiltonian structure of vorticity/streamfunction theories is well-known (see for example Shepherd (1990)), however the geometry of the Monge-Ampere equation, convex analysis and their application to atmospheric flows offers a new perspective on balanced systems.

It is natural to develop the structure of infinite-dimensional systems in analytical mechanics from those of point particles. This approach is adopted by Salmon (1988b) and Shepherd (1990), and therefore we will not expand upon these matters here. It is sufficient for our present purposes to note that there are applications of finite dimensional systems in fluid dynamics that form a useful approximation to the continua and models that exploit these ideas have been developed. Of particular interest are those with structures familiar from analytical mechanics (see, for exam-

ple Purser (1988) and also Shutts & Cullen (1987)). Apart from of a brief review of functional methods in the next section the body of the geometry and analysis is presented without introduction. The reader may take the view that this would be an appropriate opportunity for a presentation of an extensive introduction to the background material, however there are an increasing number of review articles available. Schutz (1980) provides a very readable introduction to the necessary background mathematics at the advanced undergraduate/graduate level. Sewell & Roulstone (1992) discuss of some of the relevant features of canonical transformations and Legendre transformations. See Salmon (1988b) and Shepherd (1990) for introductions to Hamiltonian methods in fluids and Marsden's lectures (Marsden (1991)), for a discussion of symplectic methods in numerical models (some of the introductory material presented in §(5) follows this work).

The paper is organized as follows: In section two we give a brief review of the definitions of Hamiltonian systems with an emphasis on the infinite-dimensional cases. In section three the SG model and the Legendre transformation, under which the equations take a particularly simple form, are discussed. We then proceed in section four to describe the Hamiltonian structure of the equations and discuss the symmetries and conservation laws. In particular, we show how the symplectic structure (the conserved geometry) of a Hamiltonian system, the crucial locally conserved nonlinear balance, is represented by conservation of vorticity on fluid particles. We address the problem of formulating a rigorous approach to the subject (*c.f.* Olver (1982) and Marsden & Weinstein (1983)), with regard, in particular, to the definition of functional derivatives and closure conditions on the symplectic form. Finally,

in section five we summarize with a discussion of the applications of this work in numerical modelling.

2 Hamiltonian methods and symplectic geometry.

2.1 Preliminaries

The equations of fluid dynamics whether written in terms of Eulerian coordinates or Lagrangian labels are continuous and thus represent infinite-dimensional dynamical systems. In what follows we will be content with the body of the theory of functional analysis rather than absolute rigor. The reason for adopting such an approach is twofold. Firstly the subject matter. Lagrangian SG theory is applicable to flows with discontinuities and the problem of extending the analysis to such solutions presents a considerable challenge. Secondly, our primary aim is to establish the existence of a structure that in practice will be studied within the context of a finite-dimensional numerical model. However it is appropriate to remind ourselves of the basic functional methods and *formal* structure at this stage.

We begin with a discussion of a typical evolution problem. Consider the following system of autonomous evolution equations for a fluid with the configuration represented by a generalized coordinate $\mathbf{x}$, and velocity $\mathbf{u}$:

$$\frac{\partial u^i(t,\mathbf{x})}{\partial t} = F^i(\mathbf{u},\mathbf{x}) \ .$$

Here, $\mathbf{x} \in \Gamma \subset \mathbf{R^n}$ for some integer n. (Index or boldface vector notation, and the summation convention will be used throughout.) The F^i are general nonlinear (partial) differential or integral operators on $\mathbf{u}$. Specifically the F^i may be any functions of the following:

i) $\mathbf{u}$ and $\mathbf{x}$,

ii) derivatives of the u^i's with respect to the x^i's,

iii) $\int_\Gamma K(\mathbf{x} \mid \hat{\mathbf{x}}) f(\mathbf{u})\, d\gamma$, where f is some function, $d\gamma$ is the volume element for $\Gamma \subset \mathbf{R^n}$, and the kernel K is independent of $\mathbf{u}$.

We will not be concerned here with specific auxiliary conditions necessary for the existence and uniqueness of solutions, but suppose solutions exist and are elements of some vector space $\mathcal{V}$, over $\mathbf{R}$ (to be specified shortly), that is equipped with the inner product

$$< f \mid g > = \int_\Gamma fg\, d\gamma \ .$$

In Hamiltonian fluid dynamics certain functionals arise from *densities* defined on $\mathcal{V}$ or *phase space*. This is a consequence of the system being continuous. To clarify this point, consider for the moment a finite-dimensional system consisting of two point particles moving under the influence of an external potential $V(r^i)$, r^i being the position vector with respect to some origin of the i^{th} particle. The total energy for the system is the sum of the kinetic and potential energies of the individual particles

$$E = \sum_i \frac{\dot{r}^{i2}}{2} + V(r^i) \ .$$

To generalize the idea to a collection of an infinite number of particles then the sum over the particles would be replaced by an integral over the labelling coordinates,

thus producing a functional of $\dot{\mathbf{r}}$ and $\mathbf{r}$, the so-called energy density. We will require these ideas for our purposes and therefore to this end we define a vector space, Ξ, (over $\mathbf{R}$) of differentiable functionals that have the form

$$\mathcal{G}[\mathbf{u}] = \int_\Gamma G(\mathbf{u}, \mathbf{x})\, d\gamma$$

where $\mathcal{G}$ is an operator on Ξ. Functional differentiation is defined by the usual Gateaux derivative

$$\frac{d}{d\epsilon}\mathcal{F}[u^i + \epsilon\varpi]\Big|_{\epsilon=0} = \left\langle \frac{\delta\mathcal{F}}{\delta u^i} \middle| \varpi \right\rangle \tag{1}$$

where the variation δ, is taken with respect to functions ϖ that vanish on $\partial\Gamma$. Equation (1) defines the functional derivative $\dfrac{\delta\mathcal{F}}{\delta u^i}$, which, in general, is nonlinear in the u^i.

Example.

Consider the Hamiltonian functional $\mathcal{H}[\mathbf{u}, \mathbf{r}]$ that governs the evolution of the shallow water model (Salmon 1985)

$$\mathcal{H}[\mathbf{u}, \mathbf{r}] = \frac{1}{2}\int (\mathbf{u}^2 + gh(\mathbf{r}))\, d\gamma$$

where h($\mathbf{r}$) is the depth of the columnar flow, g the acceleration due to gravity and the measure $d\gamma$ is over the labelling coordinates. Using (1) we obtain

$$\begin{aligned}\frac{d}{d\epsilon}\mathcal{H}\left[u^i + \epsilon\varpi\right]\Big|_{\epsilon=0} &= \int d\gamma \frac{d}{d\epsilon}\left(H(u^i) + \frac{1}{2}\frac{\partial H}{\partial u^i}\epsilon\varpi + \mathcal{O}(\epsilon^2\varpi^2)\right)\Big|_{\epsilon=0} \\ &= \int d\gamma\, \frac{\partial H}{\partial u^i}\varpi\end{aligned}$$

where H represents the integrand of the functional $\mathcal{H}$. Thus with $\varpi = 0$ on $\partial\Gamma$, then

$$\frac{\delta\mathcal{H}}{\delta u^i} = \frac{\partial H}{\partial u^i}\ .$$

2.2 Structure of Phase Space

The material presented in this subsection is necessary for an understanding of the structure of differential equations of the Hamiltonian type. It is included because we will wish to draw attention to significant limitations which arise if the body of conventional theory is assumed to apply to the SG equations. However the reader may wish to skip to §(3) and follow the essential results in the remainder of the work without a detailed appreciation of this subsection.

The evolution of a classical physical system (for example, a fluid) can be described in terms of a curve $\xi(t)$ (parametrized by some smooth variable t), in phase space. There are two structures that enter the definition of phase space and encode the *kinematics* of the system. The configuration space is described by a differentiable manifold $\mathcal{P}$ with an appropriate topology, together with an antisymmetric bilinear operation $\{\ ,\ \}$ on the space of C^∞ functions denoted by $\check{\mathcal{S}}(\mathcal{P})$, from $\mathcal{P}$ to $\mathbf{R}$, such that the operation

$$L_{\mathcal{H}}(\mathcal{F}):\ \check{\mathcal{S}}(\mathcal{P}) \otimes \check{\mathcal{S}}(\mathcal{P}) \mapsto \check{\mathcal{S}}(\mathcal{P})$$

defined by

$$L_{\mathcal{H}}(\mathcal{F}) = \{\mathcal{F},\ \mathcal{H}\} \tag{2}$$

satisfies the following properties:

i) $\{\mathcal{F},\ \mathcal{H}\}$ is bilinear in $\mathcal{F}$ and $\mathcal{H}$.

ii) $\{\mathcal{F},\ \mathcal{H}\} = -\{\mathcal{H},\ \mathcal{F}\}$ for $\mathcal{F},\ \mathcal{H} \in \check{\mathcal{S}}(\mathcal{P})$

iii) the Jacobi condition,

$\{\mathcal{E},\ \{\mathcal{F},\ .\mathcal{H}\}\} + \{\mathcal{F},\ \{\mathcal{H},\ \mathcal{E}\}\} + \{\mathcal{H},\ \{\mathcal{E},\ \mathcal{F}\}\} = 0$ for every $\mathcal{E},\ \mathcal{F},\ \mathcal{H},\ \in \check{\mathcal{S}}(\mathcal{P})$

iv) the Leibnitz' rule,

$$\{\mathcal{E}\mathcal{F}, \mathcal{H}\} = \mathcal{E}\{\mathcal{F}, \mathcal{H}\} + \mathcal{F}\{\mathcal{E}, \mathcal{H}\} .$$

We identify the pair $(\mathcal{P}, \{\ ,\ \})$ with Ξ. The second condition requires that the operator $\{\ ,\ \}$ be anti-self-adjoint with respect to the inner product on Ξ. The Leibnitz' rule means that the operation $L_{\mathcal{H}}(\mathcal{F})$ is that of differentiation by a vector field, which we also (for the moment) denote by $L_{\mathcal{H}}$. The Jacobi identity means that the operation $\{\ ,\ \}$ is a Lie algebra structure on $\check{S}(\mathcal{P})$ and that this structure is *preserved* by the flow of $L_{\mathcal{H}}$. In other words, for all t

$$\{\mathcal{F} \circ \varphi, \mathcal{G} \circ \varphi\} = \{\mathcal{F}, \mathcal{G}\} \circ \varphi$$

where φ is the time t- map for the *flow* $X_{\mathcal{H}}$, generated by $L_{\mathcal{H}}$. That is

$$X_{\mathcal{H}} = L_{\mathcal{H}} .$$

The flow satisfies the differential equations determined by $L_{\mathcal{H}}$

$$\dot{z}(t) = X_{\mathcal{H}} .$$

where $z(t)$ represents an observable. This flow is called the *Hamiltonian flow*, and $\mathcal{H}$ is called its *generating function* or *Hamiltonian*. The Hamiltonian is the map

$$\mathcal{H} : \mathcal{P} \mapsto \mathbf{R} ,$$

and encodes the *dynamics*. The evolution equations may be written in terms of this structure as

$$\frac{d}{dt}(\mathcal{F} \circ \varphi) = \{\mathcal{F}, \mathcal{H}\} \circ \varphi$$

or as the time derivative commutes with the time t- map

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\} . \tag{3}$$

Before proceeding with a definition of a Hamiltonian system, we will examine the structure of the system developed thus far. The conditions (i) and (iv) imply the existence of a tensor $\mathbf{J}$ on $\mathcal{P}$, assigning to each point $z \in \mathcal{P}$ a linear map between the cotangent space (denoted $\mathcal{T}^*$) and the tangent space ($\mathcal{T}$)

$$\sharp : \mathcal{T}_z^*\mathcal{P} \mapsto \mathcal{T}_z\mathcal{P}$$

such that

$$\{\mathcal{F},\, \mathcal{H}\}(z) \;=\; \langle \mathbf{J}(z) \cdot \mathbf{d}\mathcal{F}(z),\, \mathbf{d}\mathcal{H}(z) \rangle \quad .$$

Here $\langle\ ,\ \rangle$ denotes the natural pairing between vectors and covectors (forms), and $\mathbf{d}$ the exterior derivative (Arnol'd (1989)). As we are concerned with a tensor operator we have indicated the existence of the map at each point z. Because of (ii), $\mathbf{J}$(z) is antisymmetric. Let z^i, $i = 1,...,n$ denote coordinates on $\mathcal{P}$, then (2) becomes

$$\{F,\, H\} \;=\; \frac{\partial F}{\partial z_i} J^{ij} \frac{\partial H}{\partial z_j}$$

or in the infinite-dimensional case

$$\{\mathcal{F}\ ,\ \mathcal{G}\} \;=\; \int_\Gamma \frac{\delta \mathcal{F}}{\delta z_i} J^{ij} \frac{\delta \mathcal{G}}{\delta z_j}\ d\gamma \quad . \tag{4}$$

From (4) we note

$$\{\mathcal{F}\ ,\ \mathcal{G}\} \;=\; \left\langle \frac{\delta \mathcal{F}}{\delta z_i} \middle|\ J^{ij}\ \frac{\delta \mathcal{G}}{\delta z_j} \right\rangle$$

which is an expression for the Poisson Bracket that is especially useful in formal manipulations involving distributions.

Definition 1 *Let $\mathcal{P}$ be a manifold and Ω a two-form on $\mathcal{P}$. The pair $(\mathcal{P}, \Omega)$ is called a symplectic manifold* [1] *if Ω satisfies*

i) $\mathbf{d}\Omega = 0$ *(i.e. Ω is closed)*

ii) Ω is nondegenerate.

(See Arnol'd (1989), Olver (1982), for definition and further discussion.) If $(\mathcal{P}, \Omega)$ is a symplectic manifold, define the Poisson bracket operation $\{\ ,\ \}$ by

$$\{\mathcal{F}, \mathcal{H}\} = \Omega(X_{\mathcal{F}}, X_{\mathcal{H}})$$

where $X_{\mathcal{F}}$ is the vector field generated by the function $\mathcal{F}$ on $\mathcal{P}$. This construction makes $(\mathcal{P}, \{\ ,\ \})$ into a Poisson manifold. (That is, a manifold with a Lie algebra structure on the space of differentiable functions.) Thus, in other words

Proposition 1 *Every symplectic manifold is Poisson.*

The converse is not true; for example the zero (degenerate) bracket makes any manifold Poisson. In our application here we need to distinguish between Poisson and symplectic manifolds as the former arise in the Eulerian kinematics of fluids.

The symplectic two-form Ω may expressed in terms of a (local) coordinate basis of one-forms $\mathbf{d}z^i$

$$\Omega = \frac{1}{2} K_{ij}\, \mathbf{d}z^i \wedge \mathbf{d}z^j \tag{5}$$

where $\wedge$ is the exterior product. K is the inverse of J, $K = J^{-1}$. It should be noted that one occasionally finds J referred to as the symplectic structure of a system,

[1] The term *symplectic* comes from the Greek and was adopted by Hermann Weyl as a substitute for the Latin *complex*.

when, in fact it is the coefficient K. The cosymplectic tensor field written in terms of the vector basis $\frac{\partial}{\partial z^i}$ is

$$\Theta = \frac{1}{2} J^{ij} \frac{\partial}{\partial z^i} \wedge \frac{\partial}{\partial z^j} \tag{6}$$

and may be regarded as the fundamental object determining a Poisson structure, rather than the Poisson bracket, which is easily recovered from Θ

$$\{\mathcal{F}, \mathcal{G}\} = \langle \mathbf{d}F \wedge \mathbf{d}G | \, \Theta \rangle$$

where $\mathbf{d}F = \Omega(X_{\mathcal{F}})$ (and similarly for $\mathbf{d}G$), is the one-form which corresponds under the map $\flat : \mathcal{T}\mathcal{P} \mapsto \mathcal{T}^*\mathcal{P}$, determined by Ω, to the vector field $X_{\mathcal{F}}$.

2.3 Hamiltonian Systems

We are now in a position to define a Hamiltonian system.

Definition 2 *A Hamiltonian system consists of a Poisson manifold, that is the manifold $\mathcal{P}$ together with the bilinear operation $\{\ ,\ \}$ on $\mathcal{P}$ and a function $\mathcal{H}$ on $\mathcal{P}$ called the Hamiltonian that generates the evolution of the system according to (3).*

In particular if the matrix J^{ij} takes the following form

$$J^{ij} = \begin{pmatrix} 0^n & 1^n \\ -1^n & 0^n \end{pmatrix} \tag{7}$$

with 0^n and 1^n being the $n \times n$ zero and identity matrices, then the system is said to be *canonical.* A transformation of the phase space coordinates that preserves the form (7) is called a *canonical transformation.* To make this clear, consider a change of coordinates $z^i \mapsto f^i(z^j)$, then the equations satisfied by f are

$$\dot{f}^i = \left\langle A^i_j \middle| J^{jk} \frac{\delta \mathcal{H}}{\delta z^k} \right\rangle = \left\langle A^i_j \middle| J^{jk} A^{l\mathbf{T}}_k \frac{\delta \mathcal{H}[z(f)]}{\delta f^l} \right\rangle$$

where A^i_j is the matrix of derivatives $\dfrac{\partial f^i}{\partial z^j}$ and $A^{i\mathbf{T}}_j$ is the transpose of A^i_j. The new equations will be Hamiltonian *iff* $\mathrm{AJA}^{\mathbf{T}} = \mathrm{J}$, that is, the transformation must preserve the canonical (cosymplectic) structure.

In this paper we will consider systems of partial differential equations that may be written in the form

$$\frac{\partial \omega}{\partial t} = \mathcal{J}\Delta(\mathcal{H})$$

where $\mathcal{J}$ is, in general, a skew adjoint matrix of (pseudo-) differential operators, $\mathcal{H}[\omega]$ is the Hamiltonian functional and Δ denotes the variational derivative with respect to ω. (These considerations are entirely formal as the Sobolev subspace of L^2 under consideration will not be specified.) In addition, $\mathcal{J}$ explicitly depends on the function ω and its derivatives and therefore a closure condition on the associated symplectic structure must hold. This condition is the infinite-dimensional analogue of Darboux' theorem (Arnol'd (1989)) giving the necessary and sufficient conditions for a variable skew-symmetric matrix to be equivalent, via a change of coordinates, to the standard symplectic matrix (7). In infinite dimensions, however, the degeneracies of $\mathcal{J}$ preclude any easily defined change of coordinates to a standard form. For the Euler equations these problems have been examined by Olver (1982), and the reader is referred to that work for further details.

3 Semi-Geostrophic Dynamics

3.1 Equations of motion

The three-dimensional Boussinesq equations of semi-geostrophic theory given by Hoskins & Draghici (1977) (see also Purser & Cullen (1987)) on an f-plane can be summarized as follows:

$$\left.\begin{aligned} \frac{Du_g}{Dt} - f(v - v_g) &= 0 \\ \frac{Dv_g}{Dt} + f(u - u_g) &= 0 \end{aligned}\right\} \tag{8}$$

$$\frac{D\theta}{Dt} = 0 \tag{9}$$

$$\nabla_x \cdot \mathbf{u} = 0 \tag{10}$$

$$\nabla_x \phi = \left(f v_g, -f u_g, \frac{g\theta}{\theta_0} \right)$$

where

$$\left.\begin{aligned} \mathbf{u} &\equiv (u, v, w) \\ \mathbf{u}_g &\equiv (u_g, v_g, 0) \\ \mathbf{x} &\equiv (x, y, z) \\ \nabla_x &\equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \end{aligned}\right\} \tag{11}$$

and

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla_x \ .$$

Defining transformed coordinates

$$\mathbf{X} \equiv (X, Y, Z) \equiv \left[x + \frac{v_g}{f}, y - \frac{u_g}{f}, \frac{g\theta}{f^2 \theta_0} \right] \tag{12}$$

then (8) and (9) may be replaced by

$$\frac{D\mathbf{X}}{Dt} = \mathbf{u}_g \tag{13}$$

that is, the motion in transformed coordinates is exactly geostrophic. The Jacobian

$$q = \frac{\partial(X, Y, Z)}{\partial(x, y, z)}$$

defines a consistent form of the Ertel potential vorticity in SG, satisfying

$$\frac{Dq}{Dt} = 0 \ . \tag{14}$$

3.2 The Legendre Transform

(8) and (13) have a particular duality structure. The vector $\mathbf{X}$ may be expressed as the gradient of some function $P(\mathbf{x})$

$$\mathbf{X} = \nabla_x P \ .$$

Within an arbitrary additive constant this function is uniquely defined by

$$P = \frac{1}{f^2}\phi + \frac{1}{2}(x^2 + y^2) \ .$$

Define

$$\mathbf{Q}(\mathbf{x}) \equiv \nabla_x \mathbf{X}$$

then $\mathbf{Q}$ is the Hessian of P with respect to $\mathbf{x}$:

$$\mathbf{Q} = \nabla_x \nabla_x P = \mathrm{Hes}(P) \ .$$

$\mathbf{Q}$ is symmetric, so when it is non-singular its inverse exists, and

$$\mathbf{Q}^{-1} = \nabla_X x$$

where

$$\nabla_X \equiv \left(\frac{\partial}{\partial X}, \frac{\partial}{\partial Y}, \frac{\partial}{\partial Z}\right)$$

is symmetric also, implying that $\mathbf{x}$ is the gradient of some function $R(\mathbf{X})$:

$$\mathbf{x} = \nabla_X R \ . \tag{15}$$

To determine R, note that

$$dR = \mathbf{x} \cdot d\mathbf{X} = d(\mathbf{x} \cdot \mathbf{X}) - \mathbf{X} \cdot d\mathbf{x} = d(\mathbf{x} \cdot \mathbf{X} - P)$$

so that R is given to within an additive constant by

$$R(\mathbf{X}) = \mathbf{x} \cdot \mathbf{X} - P(\mathbf{x})$$

which is the expression for the *Legendre transform* between R and P. From (10) and (14) we infer that the motion is non-divergent in $\mathbf{X}$-space:

$$\nabla_X \cdot \mathbf{u}_g = 0$$

and therefore, being constrained to Z-surfaces, is expressible in terms of a stream-function

$$(u_g, \ v_g) = \frac{1}{f}\left(-\frac{\partial \Psi}{\partial Y}, \ \frac{\partial \Psi}{\partial X}\right) \ .$$

From (12) and (15)

$$\left.\begin{aligned} u_g &= f\left(\frac{\partial R}{\partial Y} - Y\right) \\ v_g &= -f\left(\frac{\partial R}{\partial X} - X\right) \end{aligned}\right\} \tag{16}$$

and hence the simplest form for Ψ is given by

$$\Psi = f^2\left(\frac{1}{2}(X^2 + Y^2) - R(\mathbf{X})\right) \ . \tag{17}$$

The particular duality structure described above is but *one* realization of a *quartet*

of Legendre transformations described in Chynoweth & Sewell (1989). In addition to the functions R and P there are two more, namely T and S where

$$\begin{aligned} T &= T[\tilde{\mathbf{x}},\, Z] \\ S &= S[\tilde{\mathbf{X}},\, z] \end{aligned}$$

with $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{X}}$ have two components $(x,\, y)$ and $(X,\, Y)$ respectively. The complete picture is as follows

$$\left.\begin{aligned} T + R = \tilde{\mathbf{x}} \cdot \tilde{\mathbf{X}}, \quad \tilde{\mathbf{X}} &= \frac{\partial \mathbf{T}}{\partial \tilde{\mathbf{x}}}, \quad \tilde{\mathbf{x}} = \frac{\partial \mathbf{R}}{\partial \tilde{\mathbf{X}}}, \\ R - S = Zz, \quad z &= \frac{\partial R}{\partial Z}, \quad Z = -\frac{\partial S}{\partial z}, \\ S + P = \tilde{\mathbf{X}} \cdot \tilde{\mathbf{x}}, \quad \tilde{\mathbf{x}} &= \frac{\partial \mathbf{S}}{\partial \tilde{\mathbf{X}}}, \quad \tilde{\mathbf{X}} = \frac{\partial \mathbf{P}}{\partial \tilde{\mathbf{x}}}, \\ P - T = zZ, \quad Z &= \frac{\partial P}{\partial z}, \quad z = -\frac{\partial T}{\partial Z}. \end{aligned}\right\} \tag{18}$$

We may use the quartet to express the equations of motion (8) and (9) in various different ways (Chynoweth & Sewell (1991)). There are two forms that will be especially useful in our examination of the kinematics. The first is the use of the momentum/entropy variables $(X,\, Y,\, Z)$ which gives the following system:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \dot{X}\frac{\partial}{\partial X} + \dot{Y}\frac{\partial}{\partial Y} + \dot{Z}\frac{\partial}{\partial Z} \tag{19}$$

with $\dot{} = \dfrac{D}{Dt}$.

$$\dot{q} = 0 \quad \text{where} \quad q = \rho^{-1} = (\det |\mathrm{Hes}(R)|)^{-1} \tag{20}$$

and

$$\left.\begin{aligned} \dot{X} &= \frac{\partial R}{\partial Y} - \frac{1}{f}Y \\ \dot{Y} &= -\frac{\partial R}{\partial X} + \frac{1}{f}X \end{aligned}\right\} \tag{21}$$

$$\dot{Z} = 0 \quad . \tag{22}$$

(22) simplifies (19). The operator (19) with (22) allows (20) to be rewritten in the form

$$\frac{\partial q}{\partial t} + \frac{\partial (q\dot{X})}{\partial X} + \frac{\partial (q\dot{Y})}{\partial Y} = 0$$

after also using

$$\frac{\partial \dot{X}}{\partial X} + \frac{\partial \dot{Y}}{\partial Y} = 0 \ .$$

If $q \neq 0$ we find that (20)-(22) similarly imply

$$\frac{\partial}{\partial t}\left(\frac{1}{q}\right) + \frac{\partial}{\partial X}\left(\frac{\dot{X}}{q}\right) + \frac{\partial}{\partial Y}\left(\frac{\dot{Y}}{q}\right) = 0$$

which will be the starting point for our discussion of the noncanonical Hamiltonian structure in the next section.

Note that the relationship between the vertical coordinate Z and the thermodynamic variables for an ideal gas is given by

$$Z = \frac{g\theta}{\theta_0}$$

where

$$\theta[S] = \frac{1}{R}\kappa^{1/\gamma} p_0^{(\gamma-1)/\gamma}$$

with R, $\gamma = \frac{c_p}{c_v}$ constants, and

$$\kappa[S] = R \exp(S - s)/c_v \ .$$

S is the entropy and s a constant.

The other system of equations is obtained by using the T-function, and gives a physical space/isentropic description $(x,\ y,\ Z)$.

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \dot{x}\frac{\partial}{\partial x} + \dot{y}\frac{\partial}{\partial y} + \dot{Z}\frac{\partial}{\partial Z}$$

with $\dot{\cdot} = \dfrac{D}{Dt}$. Again we find the conservation law

$$\dot{q} = 0 \quad \text{where} \quad q = -\begin{vmatrix} \dfrac{\partial^2 T}{\partial x^2} & \dfrac{\partial^2 T}{\partial x \partial y} \\ \dfrac{\partial^2 T}{\partial y \partial x} & \dfrac{\partial^2 T}{\partial y} \end{vmatrix} \left(\frac{\partial^2 T}{\partial Z^2}\right)^{-1}$$

with

$$\left.\begin{aligned} \frac{D}{Dt}\left(\frac{\partial T}{\partial x}\right) &= y - \frac{1}{f}\frac{\partial T}{\partial y} \\ \frac{D}{Dt}\left(\frac{\partial T}{\partial y}\right) &= -x + \frac{1}{f}\frac{\partial T}{\partial x} \end{aligned}\right\}$$

and

$$\dot{Z} = 0$$

4 Hamiltonian Structure

4.1 Lagrangian Kinematics

The equations of motion as written in (13) or (21) possess a canonical Hamiltonian structure in the sense of (3), (4) and (7). Consider "sufficiently smooth" solutions to (21) and the Hamiltonian functional

$$\mathcal{H}[\mathbf{X}] = \int_\Gamma d\gamma\, f^2 \left(\frac{1}{2}\left(X^2 + Y^2\right) - R(\mathbf{X}) \right) \tag{23}$$

where $d\gamma$ is the measure over the Lagrangian particle labelling coordinates $(a,\ b,\ c)$, assigned at $\tau = 0$

$$\mathbf{X}(\mathbf{a},\ \tau)\ :\ \mathbf{X}(\mathbf{a},\ 0) = \mathbf{a}\ .$$

Within this framework time is labelled τ. $\dfrac{\partial}{\partial t}$ means that $\mathbf{X}$ are held fixed while $\dfrac{\partial}{\partial \tau}$ means that $\mathbf{a}$ are held fixed. This gives $\dfrac{\partial}{\partial \tau} = \dfrac{D}{Dt}$. The Lagrangian mass label is chosen to incorporate the mass density ρ via

$$\rho d\mathbf{X} = d(\text{mass}) = d\mathbf{a}\ .$$

With this choice ρ becomes the Jacobian of the map

$$(\mathbf{a}) \mapsto (\mathbf{X})$$

that is

$$\rho(\mathbf{X},\ \tau) = \frac{\partial(\mathbf{a})}{\partial(\mathbf{X}(\mathbf{a},\ \tau))}\ .$$

This map gives the fluid flow. In §(3.1) (and in the literature referred to therein) the potential vorticity q, and thus by implication the dual space mass-density ρ were given by the ratio of the measures in x-space and (dual) $\mathbf{X}$-space. Thereby it is

implicit in that description that there is a constant mass-weighting given by

$$\frac{\partial(\mathbf{x})}{\partial(\mathbf{a})}$$

and set equal to unity. In this paper (and as in Shutts (1989)) the dependence on the particle label coordinates will be explicit.

Proposition 2 *The equations of motion (13) take the form*

$$\frac{\partial \mathbf{X}}{\partial \tau} = \{\mathbf{X}, \mathcal{H}\}_C$$

where $\{\ ,\ \}_C$ *is given by*

$$\{\mathcal{F}, \mathcal{G}\}_C = \int_\Gamma d\gamma \left(\frac{\delta \mathcal{F}}{\delta X(\mathbf{a})} \frac{\delta \mathcal{G}}{\delta Y(\mathbf{a})} - \frac{\delta \mathcal{F}}{\delta Y(\mathbf{a})} \frac{\delta \mathcal{G}}{\delta X(\mathbf{a})} \right) .$$

Proof

Calculating the functional derivatives we find

$$\begin{aligned} \frac{\delta \mathcal{H}}{\delta X} &= f^2 \left(X - \frac{\partial R}{\partial X} \right) = v_g f \\ \frac{\delta \mathcal{H}}{\delta Y} &= f^2 \left(Y - \frac{\partial R}{\partial Y} \right) = -u_g f \end{aligned}$$

and using $\{\mathbf{X}_1, \mathbf{X}_2\}_C = \delta(\mathbf{X}_1 - \mathbf{X}_2)$, we obtain the equations of motion

$$\left.\begin{aligned} \frac{\partial X}{\partial \tau} &= -\frac{1}{f} \frac{\delta \mathcal{H}}{\delta Y} = u_g \\ \frac{\partial Y}{\partial \tau} &= \frac{1}{f} \frac{\delta \mathcal{H}}{\delta X} = v_g \end{aligned}\right\}$$

in agreement with (13). □

One can show that the **X**-space mass density ρ (which is the inverse of potential vorticity), is conserved

$$\{\rho,\, \mathcal{H}\}_C \;=\; 0$$

as follows.

Express ρ in functional form via the definition of the δ-function

$$\rho(\mathbf{X}(\mathbf{a})) \;=\; \int_{\hat{\Gamma}} d\hat{\gamma}\, \delta(\mathbf{a}-\hat{\mathbf{a}}) \frac{\partial(\hat{\mathbf{a}})}{\partial(\mathbf{X})} \quad .$$

With this form we calculate the variation of ρ with respect to **X**

$$\delta_{\mathbf{X}}\rho \;=\; \int_{\hat{\Gamma}} d\hat{\gamma}\, \delta(\mathbf{a}-\hat{\mathbf{a}})(-1) \left(\frac{\partial \hat{\mathbf{a}}}{\partial \mathbf{X}}\right) \frac{\partial \hat{a}^i}{\partial \mathbf{X}^j} \frac{\partial \delta X^j}{\partial \hat{a}^i}$$

where we have used

$$\delta_x \left(\frac{\partial(\mathbf{x})}{\partial(\mathbf{y})}\right) \;=\; \frac{\partial(\mathbf{x})}{\partial(\mathbf{y})} \frac{\partial y^i}{\partial x^j} \frac{\partial \delta x^j}{\partial y^i} \quad .$$

It is useful to note the identity

$$\frac{\partial}{\partial y^i} \left(\frac{\partial(\mathbf{x})}{\partial(\mathbf{y})} \frac{\partial y^i}{\partial x^j}\right) \;=\; 0$$

known as the *Piola identity*, which has been used frequently in these calculations. Thus $\dfrac{\delta\rho}{\delta\mathbf{X}}$ is given by

$$\frac{\delta\rho(\mathbf{X}(\mathbf{a}))}{\delta X^j(\hat{\mathbf{a}})} \;=\; \frac{\partial(\mathbf{X})}{\partial(\hat{\mathbf{a}})} \frac{\partial \hat{a}^i}{\partial X^j} \frac{\partial}{\partial \hat{a}^i} \left(\rho(\mathbf{X}(\hat{a}))^2 \delta(\mathbf{a}-\hat{\mathbf{a}})\right) \quad .$$

From the expression for the Hamiltonian (23) and the reciprocity relation (15) we find

$$\frac{\delta\mathcal{H}}{\delta X^j} \;=\; f^2(X^j - x^j)$$

thus the expression for the Poisson bracket is

$$\begin{aligned}
\{\rho,\, \mathcal{H}\} &= f^2 \int_{\hat{\Gamma}} d\hat{\gamma} \left(\hat{\rho}^{-1} (\hat{\rho})^i_X \frac{\partial}{\partial \hat{a}^i} \left(\hat{\rho}^2 \delta(\mathbf{a} - \hat{\mathbf{a}}) \right) (Y - y) \right. \\
&\quad \left. - \hat{\rho}^{-1} (\hat{\rho})^i_Y \frac{\partial}{\partial \hat{a}^i} \left(\hat{\rho}^2 \delta(\mathbf{a} - \hat{\mathbf{a}}) \right) (X - x) \right) \\
&= f^2 \int_{\hat{\Gamma}} d\hat{\gamma} \left((-1) \hat{\rho}^{-1} (\hat{\rho})^i_X \hat{\rho}^2 \delta(\mathbf{a} - \hat{\mathbf{a}}) \frac{\partial}{\partial \hat{a}^i} (Y - y) \right. \\
&\quad \left. + \hat{\rho}^{-1} (\hat{\rho})^i \hat{\rho}^2 \delta(\mathbf{a} - \hat{\mathbf{a}}) \frac{\partial}{\partial \hat{a}^i} (X - x) \right) \\
&= f^2 \left(-\rho \frac{\partial a^i}{\partial X} \frac{\partial}{\partial a^i} (Y - y) \,+\, \rho \frac{\partial a^i}{\partial Y} \frac{\partial}{\partial a^i} (X - x) \right) \,=\, 0 \ .
\end{aligned}$$

We have employed the shorthand notation for the Jacobian terms viz:

$$\hat{\rho} \,\equiv\, \frac{\partial(\hat{\mathbf{a}})}{\partial(\mathbf{X})}$$

and

$$\hat{\rho}^i_{\mathbf{X}} \,\equiv\, \frac{\partial \hat{a}^i}{\partial \mathbf{X}} \ .$$

Conservation of potential vorticity may be established using the procedure outlined above by noting

$$q(\mathbf{a}) \,=\, \int_{\Gamma} d\hat{\gamma} \delta(\mathbf{a} - \hat{\mathbf{a}}) \hat{\rho}^{-1}$$

and thus

$$\{q,\, \mathcal{H}\} \,=\, \int_{\hat{\Gamma}} d\hat{\gamma} \frac{\delta q}{\delta \hat{\rho}} \{\hat{\rho},\, \mathcal{H}\} \,=\, 0 \ . \tag{24}$$

Alternatively we may demonstrate by using the Lagrangian and Noether's theorem (Arnol'd 1989) to relate symmetries and conservation laws, that invariance of the Hamiltonian system with respect to the allocation of particle labels leads to the conservation law for potential vorticity. This calculation was given by Shutts (1989).

As the particle labels do not enter the Hamiltonian (23) explicitly, yet differentiation with respect to time is affected by particle relabelling we work with the Lagrangian for the SG equations. Define the Lagrangian L

$$L[\mathbf{X},\, \dot{\mathbf{X}}] \equiv \frac{f}{2}\int_\Gamma d\gamma \left(X\dot{Y} - Y\dot{X}\right) \;-\; H[\mathbf{X}] \tag{25}$$

and consider a relabelling of the particles given by

$$\left.\begin{aligned} a' &= a \;+\; \delta a(a,b,c,\tau) \\ b' &= b \;+\; \delta b(a,b,c,\tau) \\ c' &= c \;+\; \delta c(a,b,c,\tau) \end{aligned}\right\} \;. \tag{26}$$

The flow is nonhomentropic and it is convenient to let the entropy be one of the label coordinates. We therefore set $S = c$ and consider variations satisfying

$$\delta\left(\frac{\partial(a,b,S)}{\partial(x,y,z)}\right) = 0 \quad \text{and} \quad \delta S = 0 \;. \tag{27}$$

These variations correspond to a relabelling of the fluid particles within surfaces of constant entropy. Now (27) implies

$$\delta a = -\frac{\partial\psi}{\partial b}, \quad \delta b = \frac{\partial\psi}{\partial a}$$

for some $\psi(a,b,S,\tau)$. Differentiation with respect to time after a relabelling is given by

$$\left.\frac{\partial X}{\partial\tau}\right|_{(a,b,S)} = \left.\frac{\partial X}{\partial\tau}\right|_{(a',b',S)} + \frac{\partial X}{\partial a'}\frac{\partial a'}{\partial\tau} + \frac{\partial X}{\partial b'}\frac{\partial b'}{\partial\tau}$$

so that

$$\delta\left(\frac{\partial X}{\partial\tau}\right) = -\frac{\partial X}{\partial a}\frac{\partial\delta a}{\partial\tau} - \frac{\partial X}{\partial b}\frac{\partial\delta b}{\partial\tau} \;. \tag{28}$$

As remarked the Hamiltonian has no explicit dependence on the labels and thus taking the variation of the Lagrangian (25) with respect to the labels we have

$$\delta_{\mathbf{a}} L = \frac{f}{2}\int_\Gamma d\gamma \left(X\delta\dot{Y} - Y\delta\dot{X}\right)$$

which, on using (28) and integrating the action $I = \int d\tau L$, by parts using $\psi = 0$ on $\partial\Gamma$, and at the endpoints of the τ-integration

$$\frac{f}{2}\int_{\Gamma} d\gamma\, \psi \frac{\partial}{\partial\tau}\left(\frac{\partial(X,Y)}{\partial(a,b)}\right)$$

which must vanish if the system is to be unperturbed by the particle relabelling. Thus, since ψ is arbitrary

$$\frac{\partial}{\partial\tau}\left(\frac{\partial(X,Y)}{\partial(a,b)}\right) = 0$$

but

$$\frac{\partial S}{\partial\tau} = 0$$

and so

$$\frac{\partial}{\partial\tau}\left(\frac{\partial(X,Y,S)}{\partial(a,b,c)}\right) = 0$$

and as $S = S(\theta)$ this is the result we require.

4.2 Symplectic structure and particle labels

In this subsection we demonstrate that the conservation of vorticity may be related directly to the requirement of symplectic invariance with the choice of canonical coordinates X and Y. As in the case of the vanishing of the Poisson bracket (24) this approach is essentially Hamiltonian and thus the introduction of the Lagrangian is unnecessary. We express the form of the symplectic structure (5) and the cosymplectic structure (6) in terms of the canonical bases $\mathbf{d}l^i$ and $\dfrac{\partial}{\partial l^i}$. Here $l^i \leftrightarrow (a,b)$ are the particle labels on Z-surfaces and the indices are taken to run over the values 1, 2

$$2\,\langle \mathrm{d}X \wedge \mathrm{d}Y \,|\, \Theta \rangle \;=\; \int_\Gamma d\gamma \left[\frac{\partial X}{\partial a}\frac{\partial Y}{\partial b} \;-\; a \leftrightarrow b \right]$$

where $\Theta \;=\; \frac{1}{2} J^{ij} \frac{\partial}{\partial l^i} \wedge \frac{\partial}{\partial l^j}$. The integrand may be written, using (12), as

$$\frac{\partial(x,\,y)}{\partial(a,\,b)} \frac{1}{f} \left[f \;+\; \frac{\partial v_g}{\partial x} \;-\; \frac{\partial u_g}{\partial y} \;+\; \frac{1}{f} \frac{\partial(u_g,\,v_g)}{\partial(x,\,y)} \right]$$

which is just the SG vorticity normal to the Z-surface (Hoskins & Draghici (1977)). This is, therefore, an important relationship between the dynamical invariant $q\,|_Z$ and the canonical kinematic structures Θ and Ω. When we discuss numerical modelling of Hamiltonian systems in §(5) the importance of preserving kinematic invariants will be emphasized. Thus at this stage we note that a consistent numerical scheme for the SG model would be symplectic and vorticity preserving.

4.3 A numerical model

The Lagrangian formulation is central to the use of this model in simulating flows with discontinuities. However, when examined closely the algorithm for computing the solutions is inherently Eulerian in the sense that the representation of the time coordinate that enters the timestep calculation is t rather than τ. To clarify this point we examine the outline of the method as discussed by Purser & Cullen (1987) and Cullen, Norbury & Purser (1991).

In order to solve the equations of motion we seek a solution strategy based on the dual space representation. At each timestep define a *distribution* of

$$\rho(\mathbf{X}) \;=\; q^{-1}(\mathbf{x}) \;=\; \det\left(\mathbf{Q}^{-1}\right)$$

and solve the nonlinear elliptic or parabolic (Monge-Ampere) equation for R:

$$\det |\mathrm{Hes}(R)| \; = \; \rho$$

subject to the boundary conditions implied by the requirement

$$\nabla_X R \; = \; \mathbf{x} \; \in \; D$$

where D is the physical domain in x-space whose total measure μ must equal the integral of ρ in $\mathbf{X}$-space. The next step is to use Ψ derived from (17) to update the conserved density ρ, according to the advection equation

$$\frac{\partial \rho}{\partial t} \; = \; -\mathbf{u}_g \cdot \nabla_X \rho \; \equiv \; \frac{1}{f} \frac{\partial (\rho, \, \Psi)}{\partial (X, \, Y)} \; . \tag{29}$$

Thus we find the $\dfrac{\partial}{\partial t}$ operator on the left hand side. It is commonplace to find in the literature the equations of motion written in terms of vorticity/streamfunction variables. The example that we have here could be thought of as a nonlinear version of those models. A detailed examination of the application of these techniques but with an analytical approach can be found in the work of Abarbanel *et. al* (1986) and Shepherd (1990). The model is 3-dimensional despite the structure of the advection equation (29). As mentioned, at each timestep the Monge-Ampere equation is solved, providing the 3-dimensional coupling between the advection steps. It would therefore appear to be consistent to think of the model as essentially isentropic in the sense outlined in §(3.2). This picture leads us to the main result of the paper; a Hamiltonian approach to (29).

4.4 A noncanonical Hamiltonian approach to the advection equation

We make some brief remarks concerning the generalization of the results of §(2) to *noncanonical systems.* Suppose that a system has observables $\mathcal{F}$, $\mathcal{G}$, which may be functionals of canonical coordinates z^i. Thus the Poisson bracket for such a system is given by (4) with bilinear structure (7). It may be possible, via a process known as *reduction* (Marsden, Weinstein (1983)), to write the Poisson brackets (and thus the equations of motion) in terms of coordinates $\bar{z}^\alpha$ where $\alpha < i$ (Greek indices will be used on Eulerian variables), in the following manner

$$\{\mathcal{F}, \mathcal{G}\} = \int d\bar{\mathbf{z}}_1 \int d\bar{\mathbf{z}}_2 \frac{\delta \mathcal{F}}{\delta \bar{z}_{1\alpha}} \{\bar{z}_{1\alpha}, \bar{z}_{2\beta}\}_C \frac{\delta \mathcal{G}}{\delta \bar{z}_{2\beta}} . \tag{30}$$

This will lead to an expression of the form (4) but with J^{ij} more general than (7). We will show that this structure leads to an appropriate generalization of (29).

In practice the coordinates z^i are to be identified with the Lagrangian coordinates $X^i \leftrightarrow (X, Y, Z)$ while in the context of the present application $\bar{z} \leftrightarrow \rho(\bar{X}^i)$. It is the symmetry with respect to the particle relabelling that enables the kinematics of the system to be described in terms of a single observable together with a noncanonical structure. The salient feature of the theory of reduction is that the essential dynamics of a system may be described in terms of trajectories on a manifold which has a lower dimension than the dimension of the problem's original phase space. We assume there is a group G of symmetry transformations of $\mathcal{P}$ that transform $\mathcal{P}$ to itself by a canonical transformation. We use the symmetry group to generate a vector-valued conserved quantity denoted $\mathbf{M}$ and called the *momentum*

map. If the conserved quantity has a given value then we consider the set of all points in phase space where $\mathbf{M}$ has that value. We call this set the *level set* for $\mathbf{M}$. Assign the value μ to $\mathbf{M}$. Then the reduced phase space, denoted $\mathcal{P}_\mu$, is constructed as follows:

Definition 3 *$\mathcal{P}_\mu$ is the μ-level set for $\mathbf{M}$ on which any two points that can be transformed one to another by a group transformation are identified.*

For example, a rotating rigid body has an invariant angular momentum surface associated with the corresponding conservation law. The surface being the set of points in phase space that may be mapped to one another by a generator of the symmetry. In this case the essential dynamics is described by a trajectory on this surface. Another example is provided by the axisymmetric vortex theories of Shutts *et. al* (1988), Purser (1991a), and references contained therein. In these examples a single radial coordinate suffices to describe the essential dynamics of the system.

The *reduction theorem* (Marsden & Weinstein (1974)) states that

> $\mathcal{P}_\mu$ inherits the symplectic (or Poisson bracket) structure from that of $\mathcal{P}$, so it can be used as a new phase space. Also, the dynamical trajectories of the Hamiltonian $\mathcal{H}$ on $\mathcal{P}$ determine new trajectories on the reduced phase space.

For further discussion of this matter see Marsden & Weinstein (1974) and (1983). For a less abstract approach see Salmon (1988b).

In order to proceed with a version of (30) we now formulate the necessary Eulerian functionals. The density is written in functional form as

$$\begin{aligned} \rho(\bar{\mathbf{X}}) &= \int d\gamma\, \delta\left(\bar{\mathbf{X}} - \mathbf{a}\right) \frac{\partial(\mathbf{a})}{\partial(\mathbf{X})} \\ &= \int d\gamma\, \delta\left(\bar{\mathbf{X}} - \mathbf{X}(\mathbf{a})\right) \end{aligned} \tag{31}$$

where we have used the result

$$\delta(f(x))\frac{\partial f(x)}{\partial x} = \delta(x)$$

which may be established as follows:

$$\int \delta(f(x))df = \int \delta(x)dx = \int \delta(f)\frac{\partial f}{\partial x}\,dx \ .$$

With the functional form (31) we find

$$\frac{\delta\rho(\bar{\mathbf{X}})}{\delta X^i(\mathbf{a})} = \frac{\partial}{\partial X^i}\delta(\bar{\mathbf{X}} - \mathbf{X}(\mathbf{a})) \ . \tag{32}$$

The Hamiltonian is given by

$$\mathcal{H}[\rho] = \int d\bar{\mathbf{X}} f^2 \rho(\bar{\mathbf{X}}) \left(\frac{1}{2}\left(\bar{X}^2 + \bar{Y}^2\right) - R(\bar{\mathbf{X}})\right) \tag{33}$$

with functional derivative

$$\frac{\delta\mathcal{H}}{\delta\rho} = f^2\left(\frac{1}{2}\left(\bar{X}^2 + \bar{Y}^2\right) - R\right) \ . \tag{34}$$

We may now formulate the Hamiltonian structure of (29).

Theorem 1 *The equation of motion (29) may be written in the following Hamiltonian form*

$$\frac{\partial \rho(\bar{\mathbf{X}})}{\partial t} = \{\rho(\bar{\mathbf{X}}),\, \mathcal{H}\}_E$$

with

$$\{\mathcal{F},\, \mathcal{G}\}_E = -\int_\Gamma d\bar{\mathbf{X}} \frac{\delta \mathcal{F}}{\delta \rho(\bar{\mathbf{X}})} \left(\frac{\partial \left(\rho(\bar{\mathbf{X}}), \frac{\delta \mathcal{G}}{\delta \rho(\bar{\mathbf{X}})} \right)}{\partial (\bar{X},\, \bar{Y})} \right)$$

and Hamiltonian given by (33). Γ *is taken to be a union of bounded components in* $\bar{\mathbf{X}}$.

Proof

In practice the integration is performed on constant-Z cross-sections of Γ. From (30) we have

$$\{\mathcal{F},\, \mathcal{G}\}_E = \int d\bar{\mathbf{X}}_1 \int d\bar{\mathbf{X}}_2 \frac{\delta \mathcal{F}}{\delta \rho(\bar{\mathbf{X}}_1)} \{\rho(\bar{\mathbf{X}}_1),\, \rho(\bar{\mathbf{X}}_2)\}_C \frac{\delta \mathcal{G}}{\delta \rho(\bar{\mathbf{X}}_2)} \,. \qquad (35)$$

Substituting for $\frac{\delta \rho(\bar{\mathbf{X}})}{\delta \mathbf{X}}$ and using the canonical form of the bracket, the right hand side of (35) is

$$\int d\bar{\mathbf{X}}_1 \int d\bar{\mathbf{X}}_2 \frac{\delta \mathcal{F}}{\delta \rho(\bar{\mathbf{X}}_1)} \int d\bar{\mathbf{X}}\, \rho(\bar{\mathbf{X}}) \left(\frac{\partial \left(\delta(\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}), \delta(\bar{\mathbf{X}}_2 - \bar{\mathbf{X}}) \right)}{\partial (\bar{X}, \bar{Y})} \right) \frac{\delta \mathcal{G}}{\delta \rho(\bar{\mathbf{X}}_2)} \,.$$

Integrating by parts once we obtain

$$\int d\bar{\mathbf{X}}_1 \int d\bar{\mathbf{X}}_2 \int d\bar{\mathbf{X}} \frac{\delta \mathcal{G}}{\delta \rho(\bar{\mathbf{X}}_2)} \delta(\bar{\mathbf{X}}_1 - \mathbf{X}) \frac{\partial \left(\delta(\bar{\mathbf{X}}_2 - \bar{\mathbf{X}}), \frac{\delta \mathcal{F}}{\delta \rho(\bar{\mathbf{X}}_1)} \rho(\mathbf{X}) \right)}{\partial (\bar{X}, \bar{Y})}$$

which upon using the functional relationship (31) and integrating out the $\bar{\mathbf{X}}_1$ variables becomes

$$\int d\bar{\mathbf{X}}_2 \int d\bar{\mathbf{X}}\, \rho(\bar{\mathbf{X}}) \frac{\delta \mathcal{G}}{\delta \rho(\bar{\mathbf{X}}_2)} \frac{\partial \left(\delta(\bar{\mathbf{X}}_2 - \bar{\mathbf{X}}), \frac{\delta \mathcal{F}}{\delta \rho(\bar{\mathbf{X}})} \right)}{\partial (\bar{X}, \bar{Y})} \,.$$

We may perform the operation again and integrate out the $\bar{\mathbf{X}}_2$ variables to get

$$\int d\bar{\mathbf{X}}\, \rho(\bar{\mathbf{X}}) \frac{\partial\left(\frac{\delta\mathcal{F}}{\delta\rho}, \frac{\delta\mathcal{G}}{\delta\rho}\right)}{\partial\left(\bar{X}, \bar{Y}\right)} \tag{36}$$

which may be re-written for admissible functional derivatives [2] as

$$-\int d\bar{\mathbf{X}}\, \frac{\delta\mathcal{F}}{\delta\rho}\left(\frac{\partial\left(\rho, \frac{\delta\mathcal{G}}{\delta\rho}\right)}{\partial\left(\bar{X}, \bar{Y}\right)}\right) \quad . \tag{37}$$

We may identify $\mathcal{F}$ with ρ and $\mathcal{G}$ with $\mathcal{H}$ and evaluate the bracket to obtain (29). The functional derivatives we require are given by (32) and by (34). From (36), we evaluate

$$f^2 \int d\bar{X} d\bar{Y}\ \rho(\bar{\mathbf{X}}) \left(\frac{\partial\left(\frac{1}{2}\left(\bar{X}^2 + \bar{Y}^2\right) - R\right)}{\partial\bar{X}} \frac{\partial\delta\left(\bar{\mathbf{X}} - \mathbf{X}\right)}{\partial\bar{Y}} - \bar{X} \leftrightarrow \bar{Y}\right) \quad .$$

Upon integrating by parts and integrating out the variables $\bar{\mathbf{X}}$, leaves us with

$$f^2 \left(\frac{\partial\rho}{\partial X} \frac{\partial\left(\frac{1}{2}\mathbf{X}^2 - R\right)}{\partial Y} - X \leftrightarrow Y\right)$$

and thus using (15) and (16), we have

$$-f u_g \frac{\partial\rho}{\partial X} - f v_g \frac{\partial\rho}{\partial Y} \tag{38}$$

which is precisely the right hand side of the advection equation (29). □

One may note that the form of (36) means that the bracket of functionals depending on ρ alone will be in *involution* with respect to $\{\ ,\ \}_E$. The bilinear structure is identified to be

$$J^\bullet = \frac{\partial\left(\rho, \bullet\right)}{\partial\left(\bar{X}, \bar{Y}\right)} \quad .$$

[2] Appropriate boundary conditions must be satisfied. We will discuss this briefly in the following subsection.

4.5 Formal structure and boundary conditions

There are a number of points to be addressed concerning the (formal) Hamiltonian structure of the system described by theorem 1. (See also §(2.3).)

i) The properties of the bilinear operation $\{\ ,\ \}$ laid out in §(2) were for C^∞-functions on $\mathcal{P}$, while the SG solutions will involve the quantities R and P that may be only piecewise smooth (piecewise C^1). The theory of *subdifferentials* may be applied in order to obtain a derivative of such a function and the *Fenchel transform* is an appropriate generalization of the Legendre transform for such (convex) functions. However, in order to construct the Hamiltonian system in the manner described in §(2), one should address the problem of defining a functional derivative such that the properties of the Poisson manifold may be established.

ii) The integration by parts used to arrive at (37) is valid, at least in a formal sense, as the δ-function terms were integrated out at each step. However, in general the boundary conditions satisfied by the functional derivatives must be made explicit. McIntyre & Shepherd (1987) discuss a class of *admissible* functionals $\{\mathcal{A}[\varrho]\}$ satisfying

$$\frac{\partial\left(\dfrac{\delta\mathcal{A}}{\delta\varrho}\right)}{\partial s} = 0 \quad \text{on } \partial\Gamma$$

where s is the arclength on the boundary, thus enabling integration by parts to be used. They also demonstrate that the *second* functional derivatives are admissible and this enables the Jacobi identity (which involves the derivative of brackets) to be established. For general functionals that arise in SG theory we may, under certain

conditions, take $\rho = 0$ on the boundary. In general however, the boundary conditions imposed with respect to the domain in which the fluid motion takes place need to be translated into conditions on ∇R. For R convex and $\mathbf{t}$ a tangent vector to any line through the components, $\mathbf{t}.\nabla R$ must be monotonic as we move along the line. This implies $\mathbf{x}$ is monotonic as $\mathbf{X}$ moves along the line. Internal component boundaries need continuity conditions, while the external boundary of the components corresponds to the boundary in the $\mathbf{x}$ domain.

iii) In §(2.3) a brief reference was made to the closure condition on the symplectic form. The problem is to identify a symplectic 2-form for the reduced system. A rigorous treatment of this problem for the model presented in this paper using conventional techniques would not appear to be possible. By conventional, we are referring to the technique employed by Marsden & Weinstein (1983), based on a Lie group structure. For an ideal fluid (incompressible and homogeneous) in some region Λ ($\Lambda \in \mathbf{R^n}$), one chooses the configuration space to be the group of volume preserving diffeomorphisms $\mathcal{D}_{vol}$, on Λ. The phase space is $\mathcal{T}^*(\mathcal{D}_{vol})$ and there exists a Hamiltonian system (a Poisson bracket form of the vorticity equation), on the Poisson manifold $\mathcal{P}^*_{vol}$ where $\mathcal{P}_{vol}$ is the space of divergence-free vector fields on Λ parallel to $\partial\Lambda$. $\mathcal{P}_{vol}$ is the Lie algebra of $\mathcal{D}_{vol}$ and it is from this that one obtains the bracket operation. One can check that the solution curves to the vorticity equation remain on coadjoint orbits (of $\mathcal{D}_{vol}$) in $\mathcal{P}^*_{vol}$. Then the appropriate symplectic structure for the reduced system is obtained by identifying the symplectic manifold as the coadjoint orbits in $\mathcal{P}^*_{vol}$ and using an established technique (the Kirillov form) for computing the symplectic structure. From the outset, the difficulty with the SG

theory is the (apparent) lack of a Lie group structure. In the SG case the evolution may be considered as a sequence of *rearrangements* of the fluid subject to certain constraints (Cullen, Norbury & Purser (1991)). Ofcourse, it is the modelling of flows via a sequence of general rearrangements that enables one to capture discontinuities and convection.

5 Applications to the Geometric Models

There now exist efficient numerical algorithms for integrating the SG equations. The geometric ideas originating from Cullen (1983) and developed in Cullen & Purser (1984) were subsequently used in the formulation of the geometric model (Chynoweth (1987)). Recently (Purser (1991b)) a much improved and efficient version of this model has been produced thus enabling an increased resolution in the modelling of atmospheric flows. The basic algorithm was described in §(4) together with a (formal) Hamiltonian structure. We discuss now the role of the Hamiltonian structure in numerical models, leaving until the end the final question, the existence of the necessary structure in the geometric model.

The material presented in §(2) and §(4) exemplifies the geometric emphasis of modern theoretical mechanics. When studying Hamiltonian dynamics from a geometric perspective, *it is essential to distinguish the features that depend on the Hamiltonian function from those that depend only on the properties of the structure of phase space.* The classical concept of a canonical transformation is a transformation that preserves the "structure" of a Hamiltonian system. This concept may

be given a more geometric definition. The modern analogue of this concept is a *symplectic map*, a smooth map of a symplectic manifold to itself that preserves the symplectic form, or equivalently, the Poisson bracket operation. It is a goal of much current effort to develop algorithms that capture the details of the Hamiltonian structure in numerical models. These algorithms are referred to as *symplectic integrators.*

A symplectic integrator is an evolutionary finite-difference algorithm which has the property that each iteration n is given by a canonical transformation (also known as a symplectic transformation) of the phase space. The time-step size Δt is a parameter in the symplectic mapping defining the algorithm, so if this mapping approximates the Δt-time map of a Hamiltonian flow to at least positive order in Δt, the algorithm may be said to provide a finite-difference approximation of the dynamics in the usual sense. Since any number of iterations also produces a symplectic map, a symplectic integrator also preserves the Hamiltonian structure of the dynamics. With regard to the geometric model, we have learned from §(4) that the essential structure is noncanonical and therefore we devote the remainder of this paper to *reduced* symplectic integrators.

Suppose that our Hamiltonian system is invariant under the action of some group G. We expect that such a system will have conserved quantities associated with the momentum map $\mathbf{M}$. Ge & Marsden (1988) have shown that under fairly weak assumptions, a G-equivariant symplectic integrator (capturing the G-invariance of the system) exactly conserves $\mathbf{M}$, and consequently, all the constants of motion

associated with the reduction of the dynamics. The construction of symplectic momentum-conserving algorithms, requires that the level sets of the momentum map $\mathbf{M}$ remain invariant under the mapping $\varphi : \mathcal{P} \mapsto \mathcal{P}$ that represents a single iteration of the algorithm. The main result of Ge & Marsden (1988) is that if the original (not reduced) phase space is a symplectic manifold and φ is a symplectic map that is G-symmetry-preserving in the sense that

$$\varphi(gz) = g\varphi(z) \quad \forall\, z \in \mathcal{P} \text{ and } g \in G$$

then symplectic integrators that generate the timesteps in such a manner as to preserve the inherent symmetry are reduced symplectic integrators. In other words, if we denote the model variables at time t_0 by V_0 and at time t_1 by V_1 then a necessary and sufficient condition for the algorithm to be symplectic is (*c.f.* §(2.3)) $\mathrm{AJA^T} = \mathrm{J}$ where A is the matrix corresponding to the Jacobian

$$A = \frac{\partial(V_1)}{\partial(V_0)}$$

and J is given by (7). It is momentum preserving if it preserves the value of the associated conserved quantity.

Symplectic integrators do not in general conserve the energy (Hamiltonian) of a mechanical system, although there is some numerical evidence that the energy invariance remains in a reasonable range over long time intervals. In fact the energy usually remains within a bounded oscillation. One may have expected that an error would accumulate over a long time integration. Channell & Scovel (1990) report several instances of this oscillatory behaviour. It is tempting to think that one might conceive of an algorithm for preserving all the constants of motion and the

symplectic structure. However, a fairly straightforward argument due to Ge (1988), demonstrates that this cannot be the case. The argument goes as follows: Suppose $\varphi_{\Delta t}$ is a symplectic algorithm and consider the application of the algorithm to the reduced phase space. We assume that the Hamiltonian H is the only constant of motion of the reduced dynamics (*i.e.* all other constants of the system have been taken out in the reduction process). Since $\varphi_{\Delta t}$ is symplectic it must be the Δt-time map of some Hamiltonian function F. Now assume that the symplectic map $\varphi_{\Delta t}$ also conserves H for all values of Δt. Thus $\{F,\ H\} = 0$. This equation implies that F is functionally dependent on H since the "true dynamics" has no other constants of motion. The functional dependence in turn implies that their Hamiltonian vector fields are parallel, so the flow of F (the approximate solution) and the flow of H (the exact solution) must lie along identical curves in the reduced phase space; thus the flows are equivalent up to reparametrization of the curves. This result, succinctly stated, says that *it is impossible for an algorithm to simultaneously conserve the symplectic structure, the momentum map, and the Hamiltonian.* Non-symplectic algorithms that conserve both momentum and energy have been studied by Simo & Wong (1989) and Krishnaprasad & Austin (1990). This work shows that it is indeed possible to design algorithms of this sort.

The basic structure of the geometric model is symplectic (in the sense of proposition 2) and the conserved quantity, associated with the reduction to the noncanonical form used in the solution strategy, is ρ. In order for the numerics to be symplectic the time stepping algorithm used should preserve the canonical structure (7) in the following way: Let A be the matrix that leads from one timestep to another and

corresponds to the Jacobian matrix

$$A = \frac{\partial(X_1, Y_1)}{\partial(X_0, Y_0)}$$

then we require

$$\mathrm{AJA^T} = \mathrm{J} \ . \tag{39}$$

As indicated by Chynoweth & Sewell (1991) a variety of methods may be used to generate the time-Δt map and therefore (39) should be checked for each case. We then require, in order for the algorithm outlined in §(4.2) to be reduced-symplectic, that the geometric method conserve ρ. Thus, in conclusion, we note that as far as the current formulation of the model is concerned, further work is required. At the present the method conserves the energy (Hamiltonian), and as Ge's argument demonstrates, it is impossible to have a symplectic, energy and momentum conserving algorithm. Alternatively, one may attempt to retain energy conservation and formulate a ρ-preserving method that is not symplectic (using, for instance, the current predictor-corrector time stepping algorithm).

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